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'DUROV PLOT' USERS GUIDE: COMPUTER CALCULATION AND PLOTING OF DUROV DIAGRAMS FOR WATER CHEMISTRY ANALYSIS

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'DUROV PLOT' USERS GUIDE: COMPUTER CALCULATION AND
PLOTING OF DUROV DIAGRAMS FOR WATER CHEMISTRY ANALYSIS

by

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SUMMARY

The Durov trilinear plot is a method for determining changes in ground/surface water chemistry. This report describes the program 'DUROV PLOT' which undertakes the calculation and plotting of Durov diagrams. The program is written in G-BASIC for a North Star microcomputer.

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GUIDE DE L'UTILISATEUR DU PROGRAMME "DUROV PLOT":
CALCUL SUR ORDINATEUR ET TRAÇAGE DES SCHÉMAS DUROV
LORS DES ANALYSES CHIMIQUES DE L'EAU

par

D.A. Young* et T.R.C. Aston**

RÉSUMÉ

La méthode utilisant le schéma trilinéaire Durov sert à déterminer les changements chimiques dans le l'eau de surface et souterraine. Ce rapport contient donc une description du programme "DUROV PLOT" qui effectue le calcul et le traçage des schémas Durov. Ce programme est écrit en langage G-BASIC pour un micro-ordinateur North Star.

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INTRODUCTION

A number of trilinear/graphical techniques exist for the classification of ground/surface water types, Zaporozec (1). The Durov trilinear diagram allows water samples to be quickly, simply and comprehensively analysed and characterised.

The program 'DUROV PLOT' uses a modified Durov diagram to plot and present in diagrammatic form the type and trends of water chemistry samples. The program is essentially a data handling and plotting package, which greatly simplifies the analysis of water samples using the Durov technique.

To use the program it is necessary to input specific ion concentrations (milligrams/litre) determined from the chemical analysis of the water samples under consideration: sodium, potassium, calcium, magnesium, bicarbonate, sulphate and chloride.

'DUROV PLOT' was written for use on a North Star microcomputer using the North Star G-BASIC language (with associated editing and file handling software). The program is conveniently run using a 256 kB diskette and an EPSON FX100 Dot Matrix Printer. The user is expected to be familiar with the operation of microcomputers and the concept of analysing groundwater samples.

A source listing of the program is given along with examples of the input data and output format. A description of the various program segments is also given.

PROGRAM DESCRIPTION

A source listing of the program is given in Appendix A.

Line No.

10 - 140	Program Header
150 - 560	Program Preamble
570 - 580	Program Dimension Statements
590 - 890	Main Menu (Data Analysis and File Handling)
900 - 1590	Service Menu (Plotting and Printing of Results)

1600 - 1660	Data Points Plotted with Durov Diagram
1670 - 2200	Data File Search Criteria
2210 - 2430	Calculates % Ions and Durov Data Points
2440 - 2750	Prints Data Lines used in Durov Plot
2760 - 2910	Plots Points by Data File Record Number
2920 - 2980	Durov Plot Area Sectioned into Four Quadrants
2990 - 3040	Prints % Ion Concentrations
3050 - 3150	Prints Headlines for % Ion Concentrations
3160 - 3250	Counts Number of Lines in Data File
3260 - 3280	Checks for Out of Bounds Column Numbers

Lines 760 and 850 contain the term (Edit 1) which is a G-BASIC editing and file handling sub-program.

PROGRAM USE

The current version of 'DUROV PLOT' allows up to 70 data points to be plotted (dimension statement, lines 570 - 580). However, by altering the dimension statement, several hundred data points can be input and handled by the program. It should also be noted that the input data file, Table 1, is created separately and called up (chained to a G-BASIC Edit Program) by the 'DUROV PLOT' program.

'DUROV PLOT' uses a menu style operating sequence within the program, which is user friendly. The main menu, lines 720 - 770 (Appendix A), contains the following options:

```

SEARCH DATA BY LIMITS
POINT BY RECORD NUMBER PLOT
ANOTHER DATA FILE
CHAIN TO EDITOR
END SESSION

```

ID#	DATE	Na	K	Ca	Mg	ALKAL	SO4	Cl
1	830322	90	3.4	93	14	76	32	275
2	830330	81	3	89	13	76	32	256
3	830415	61	2.7	79	11	77	28	196
4	830427	65	2.8	81	12	76	30	213
5	830429	67	2.8	74	10	76	27	190
6	830512	65	2.7	72	10	77	25	175
7	830526	60	2.4	74	10	78	23	180
8	830609	57	2.4	72	10	80	22	174
9	830623	57	2.6	73	10	87	19	174
10	830706	77	2.7	88	14	92	17	245

Table 1 - Input data file used for 'DUROV PLOT'

ID#	%Na+K	%Ca	%Mg	%HCO3	%SO4	%Cl
1	46.61	46.41	6.99	19.34	8.36	71.80
2	45.16	47.85	6.99	20.88	8.79	70.33
3	41.44	51.40	7.16	25.58	9.30	65.12
4	42.16	50.37	7.46	23.82	9.40	66.77
5	45.38	48.11	6.50	26.86	9.54	63.60
6	45.22	48.10	6.68	27.80	9.03	63.18
7	42.62	50.55	6.33	27.76	8.19	64.06
8	42.01	50.92	7.07	28.99	7.97	63.04
9	41.80	51.19	7.01	31.07	6.79	62.14
10	43.36	48.43	7.71	25.99	4.80	69.21

Table 2 - Tabulated percentage ion concentrations

In addition, a service menu, lines 920 - 970 (Appendix A), contains the following options regarding output format:

DUROV PLOT
DATA LINES
PLOT ENLARGEMENT
% ION CONCENTRATION
MAIN MENU

A listing of the % Ion Concentrations obtained from the input data, Table 1, is given in Table 2. The Durov plot (service menu option) giving the location of the points in Table 1 is shown in Figure 1, while the Durov plot enlargement option is shown in Figure 2.

REFERENCES

1. Zaporozec, A. 'Graphical interpretation of water quality data'; Ground Water; Vol. 10, No. 2, pp 32 - 43; 1972.

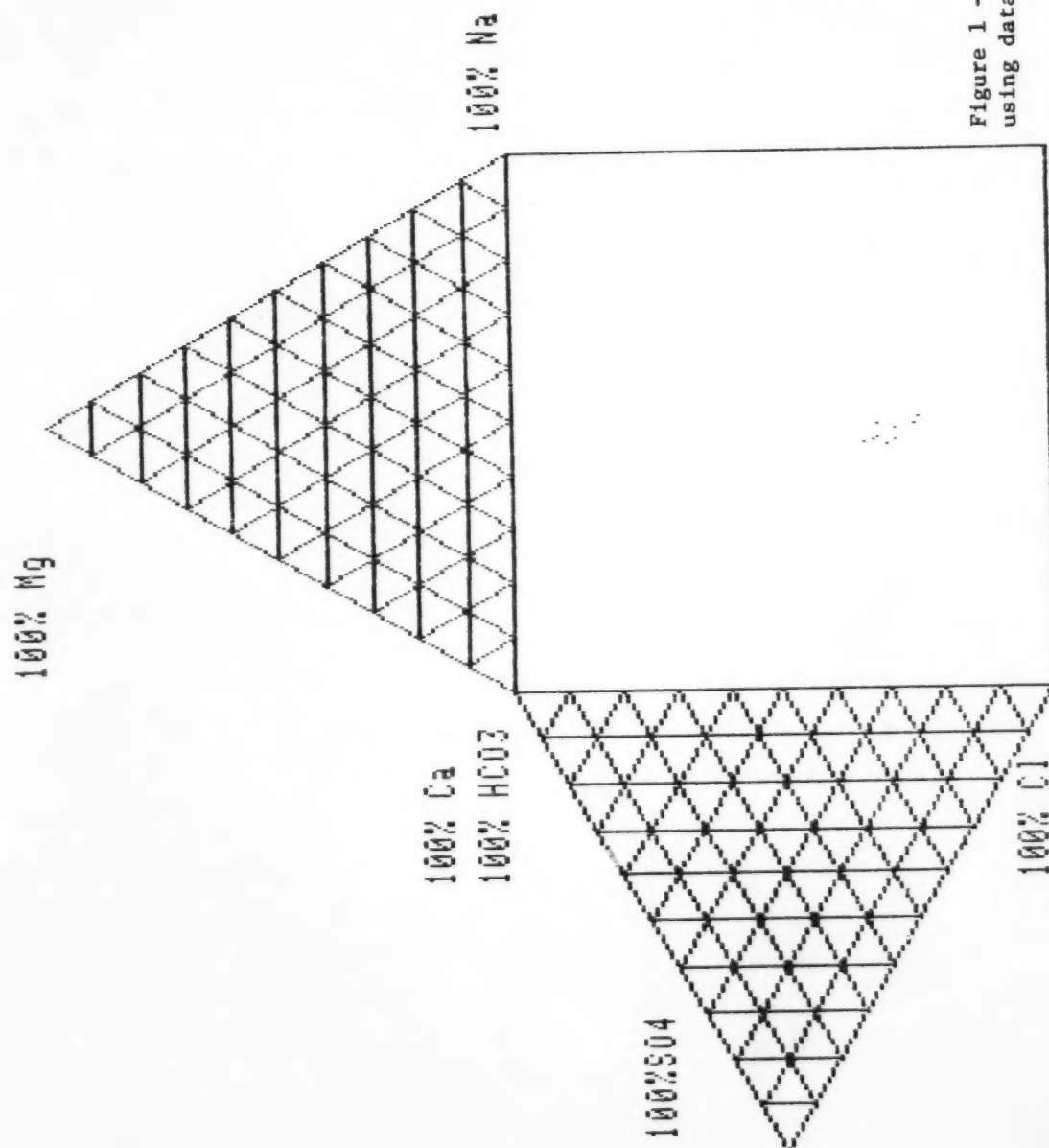
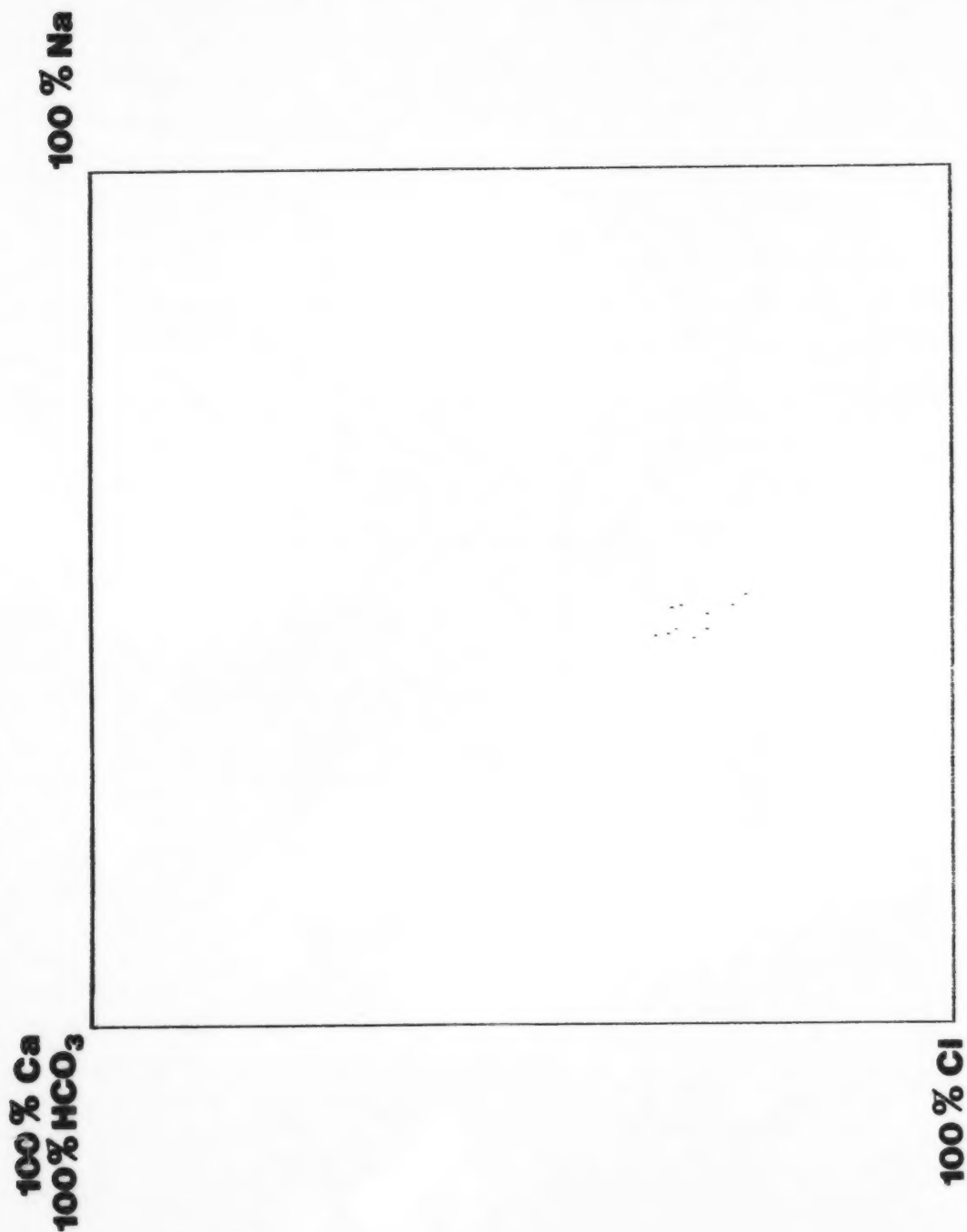


Figure 1 - Example of Durov Plot
using data given in Table 1

Figure 2 - Durov Plot enlargement option showing
data given in Table 1



A-7

APPENDIX A

```

10 REM *****
20 REM
30 REM          PROGRAM DUROV PLOT
40 REM          -----
50 REM
60 REM          Written by   David Young
70 REM                      EG-ESS-3 (Technologist)
80 REM                      Department of Energy, Mines & Resources
90 REM                      CANMET/CRL Cape Breton
100 REM                     210 George St.
110 REM                     Sydney, N.S.
120 REM                     Canada B1P 1J3
130 REM
140 REM *****
150 !CHR$(4), "DO YOU WISH TO VIEW PROGRAM DESCRIPTION (Y OR N) ", \INPUT A$
160 IF A$="Y" THEN 170 ELSE 570
170 !CHR$(4)
180 ! "          Program Operation "
190 ! "          -----"
200 ! "Input parameters -      The source file of Hydro-Chemical data is"
210 ! "                        the most important parameter to be input by the "
220 ! "                        user."
230 ! "                        :      All other input parameters are explained "
240 ! "                        by use of service menus."
250 !
260 ! "File description -      The Hydro-chemical data table is of the"
270 ! "                        following structure:"
280 ! " ID#  Date  Na  K  Ca  Mg  Alkal  SD4  Cl "
290 !
300 ! "HIT RETURN TO CONTINUE ... "\T$=INCHAR$(0)\!CHR$(4)
310 ! "Modes of operation -:"
320 ! "      (1) Search by column deliminators"
330 ! "      (2) selective search"
340 !
350 ! "(1) - This mode selects lines of data to be plotted by supplying"
360 ! "      arguments with use of numeric deliminators. As many as 9 "
370 ! "      arguments can be set at once, in any particular order."
380 ! "Example- select 2 columns for search."
390 ! "      Column Date between 820001 and 830001"
400 ! "      Column Cl  between 100meg and 200meg"
410 ! "The program will read a line a data, if the first argument holds true "
420 ! "for the information under DATE then the program passes on to the next "
430 ! "argument. If the line passes all arguments it is stored for future use"
440 ! ", if not the line is proven false and it is rejected. This process is"
450 ! "carried out for each line of data"
460 !
470 ! "(2) - The user suplys data line records to be processed. It lets the "
480 ! "user view the plotting in a graphical hybrid mode."
490 !
500 ! "HIT RETURN TO CONTINUE ... "\T$=INCHAR$(0)\!CHR$(4)
510 ! "Service Menue - In general it allows a full screen durov plot,"
520 ! "an enlargement of the plot section, hardcopy of the data lines and "
530 ! "percent ion calculations."
540 !
550 ! *****

```

```

560 ! "HIT RETURN TO CONTINUE ..." \T$=INCHAR$(0)
570 DIM P(70),P1(70),P2(70),P3(70),P4(70),P5(70)
580 DIM A(70),B(70),C(70),D(70),E(70),F(70),G(70),H(70),K(70),W(70),W1(70)
590 REM ***** MAIN MENU *****
600 REM
610 ! "*****"
620 !CHR$(4)
630 INPUT "INPUT DATA FILE NAME AND DISK DRIVE ",B$
640 GOSUB 3180\CLOSE #1
650 !CHR$(4)
660 ! "THERE IS ",D5," # OF LINES IN FILE ",B$ \FOR I=1 TO 2000\NEXT
670 IF D5=0 THEN 680 ELSE 700
680 ! "THIS FILE IS EMPTY !"
690 ! "-----" \FOR I=1 TO 2000\NEXT \GOTO 630
700 !CHR$(4)
710 !CHR$(4)
720 ! "***** MAIN MENU *****"
730 ! "(1)..... SEARCH DATA BY LIMITS "
740 ! "(2)..... POINT BY RECORD # PLOT"
750 ! "(3)..... ANOTHER DATA FILE"
760 ! "(4)..... CHAIN TO EDITOR"
770 ! "(5)..... END SESSION"
780 ! "-----"
790 INPUT "INPUT SERVICE # ?",Q
800 IF Q=1 THEN 1670 \Z6=0
810 IF Q=2 THEN 880 ELSE 820
820 IF Q=3 THEN 830 ELSE 840
830 GOTO 630
840 IF Q=4 THEN 850 ELSE 860
850 CHAIN "EDIT1"
860 IF Q=5 THEN 870 ELSE 710
870 END
880 GOSUB 2730
890 GOTO 710
900 ! "REM IF YOU REQUIRE A HARD COPY OF DUROV PLOT THEN PRESS CTRL-T"
910 !CHR$(4)
920 ! "***** SERVICE LISTING *****"
930 ! "(1).....DUROV PLOT"
940 ! "(2).....DATA LINES"
950 ! "(3).....PLOT ENLARGEMENT"
960 ! "(4).....% ION CONCENTRATION"
970 ! "(5).....MAIN MENU"
980 ! "-----"
990 INPUT "INPUT SERVICE # ",Q
1000 IF Q=1 THEN GOTO 1010 ELSE 1040
1010 GOSUB 2940
1020 GOSUB 1150\GOSUB 1280\GOSUB 1510\IF A$="Y" THEN GOSUB 1490\GOSUB 1600
1030 GOSUB 1490
1040 IF Q=2 THEN GOTO 1050 ELSE 1060
1050 GOSUB 2440
1060 IF Q=3 THEN 1070 ELSE 1100
1070 GOSUB 2940\GRAPHICS
1080 VIEWPORT 30,130,0,100\WINDOW 86.605,186.605,0,100\GOSUB 1200
1090 IF A$="Y" THEN GOSUB 1490\GOSUB 1600
1100 IF Q=4 THEN 1110 ELSE 1120
1110 GOSUB 3070\GOSUB 3010
1120 IF Q=5 THEN 1130 ELSE 910
1130 CLOSE#1\GOTO 710
1140 GOTO 900
1150 REM ***** SUB ROUTINE FOR DUROV PLOT*****

```

```

1160 REM
1170 GRAPHICS
1180 VIEWPORT 0,119,0,119
1190 WINDOW 0,200,0,200
1200 MOVE 0,50
1210 DRAW 86.605,100\DRAW 136.605,186.605\DRAW 186.605,100
1220 DRAW 86.605,100\DRAW 86.605,0\DRAW 0,50
1230 MOVE 186.605,0\DRAW 186.605,100
1240 MOVE 86.605,0\DRAW 186.605,0
1250 RETURN
1260 REM ***** FILLS DUDVS TRIANGLES *****
1270 REM
1280 J=0
1290 FOR I= 10 TO 100 STEP 10
1300 J=J+1
1310 X1=.86605*I\Y1=.57730*X1+50\X(J)=X1\Y(J)=Y1
1320 X2=86.605\Y2=100-I\X1(J)=X2\Y1(J)=Y2
1330 X3=86.605-I*.86605\Y3=50-.5773*X3\X2(J)=X3\Y2(J)=Y3
1340 X4=186.605-I\Y4=100\X3(J)=X4\Y3(J)=Y4
1350 X5 =86.605+I*.5\Y5=100+.86605*I\X4(J)=X5\Y4(J)=Y5
1360 X6 =136.605+I*.5\Y6=186.605-.86605*I\X5(J)=X6\Y5(J)=Y6
1370 NEXT
1380 FOR I=1 TO 9
1390 MOVE X(I),Y(I)\DRAW X1(10-I),Y1(10-I)\MOVE X1(10-I),Y1(10-I)
1400 DRAW X2(I),Y2(I)
1410 MOVE X(I),Y(I)\DRAW X2(10-I),Y2(10-I)
1420 MOVE X3(I),Y3(I)\DRAW X5(10-I),Y5(10-I)\MOVE X5(10-I),Y5(10-I)
1430 DRAW X4(I),Y4(I)
1440 MOVE X3(I),Y3(I)\DRAW X4(10-I),Y4(10-I)
1450 NEXT
1460 RETURN
1470 REM ***** SECTIONS PLOT *****
1480 REM
1490 MOVE 136.605,0\DRAW 136.605,100\MOVE 86.605,50\DRAW 186.605,50
1500 RETURN
1510 REM ***** LABEL AXIS *****
1520 REM
1530 MOVE 90,186\GPRINT "100% Mg"
1540 MOVE 190,100\GPRINT "100% Na"
1550 MOVE 2,70\GPRINT "100%SD4"
1560 MOVE 50,0\GPRINT "100% Cl"
1570 MOVE 50,110\GPRINT "100% Ca"
1580 MOVE 50,100\GPRINT "100% HCO3"
1590 RETURN
1600 REM ***** SUB ROUTINE FOR PLOTTING DUROV POINTS *****
1610 REM
1620 FOR X=1 TO 2
1630 POINT W1(X),W(X)
1640 NEXT
1650 A$=INCHAR$(0)
1660 RETURN
1670 REM ***** SEARCH DATA SECTION *****
1680 REM
1690 !CHR$(4)
1700 !"YOU ARE IN THE SEARCH DATA SECTION OF THE PROGRAM"

```

```

1710 !"-----"
1720 FOR I=1 TO 2000:NEXT
1730 !CHR$(4)
1740 INPUT "INPUT BY HOW MANY COLUMNS DO YOU WISH TO SEARCH ",N
1750 REM
1760 REM ** CHECKS FOR OUT OF BOUND COLUMN **
1770 REM
1780 N9=N\GOSUB 3280:IF A$="N" THEN 1790 ELSE 1810
1790 !"YOU INPUT AN OUT OF BOUNDS COLUMN #"
1800 !"-----"\GOTO 1730
1810 !CHR$(4)
1820 !"INPUT THE ORDER IN WHICH THE SEARCH IS TO CONDUCTED "
1830 RESTORE 3140
1840 FOR I=1 TO 9
1850 READ V$,V\!V," ",V$
1860 NEXT
1870 FOR I=1 TO N
1880 !CHR$(27),CHR$(61),CHR$(44),CHR$(32),
1890 INPUT "INPUT THE COLUMNS TO BE SEARCHED ",X(I)
1900 N9=X(I)\GOSUB 3280:IF A$="N" THEN 1910 ELSE 1930
1910 !"YOU INPUT AN OUT OF BOUNDS COLUMN #"
1920 !"-----"\GOTO 1890
1930 INPUT "INPUT THE LOWER NUMERIC LIMIT FOR SEARCH ",V(X(I))
1940 INPUT "INPUT THE UPPER NUMERIC LIMIT FOR SEARCH ",V1(X(I))
1950 NEXT
1960 !CHR$(4),"SEARCH IN PROCESS ..."
1970 OPEN#1,B$
1980 Z=0
1990 IF TYP(1)=0 THEN 2000 ELSE 2010
2000 GOSUB 2210\GOTO 900
2010 READ #1,A,B,C,D,E,F,G,H,K
2020 FOR I=1 TO N
2030 Y=A\ IF X(I)=1 THEN GOSUB 2170
2040 Y=B\ IF X(I)=2 THEN GOSUB 2170
2050 Y=C\ IF X(I)=3 THEN GOSUB 2170
2060 Y=D\ IF X(I)=4 THEN GOSUB 2170
2070 Y=E\ IF X(I)=5 THEN GOSUB 2170
2080 Y=F\ IF X(I)=6 THEN GOSUB 2170
2090 Y=G\ IF X(I)=7 THEN GOSUB 2170
2100 Y=H\ IF X(I)=8 THEN GOSUB 2170
2110 Y=K\ IF X(I)=9 THEN GOSUB 2170
2120 NEXT
2130 GOTO 2180
2140 REM
2150 REM ** THIS SECTION SOLVES THE SEARCH ARGUMENT ***
2160 REM
2170 IF Y<V(X(I)) OR Y>V1(X(I)) THEN 1990 ELSE RETURN
2180 Z=Z+1\Z9=1
2190 A(Z)=A\B(Z)=B\C(Z)=C\D(Z)=D\E(Z)=E\F(Z)=F\G(Z)=G\H(Z)=H\K(Z)=K\GOTO 1990
2200 REM
2210 REM ***** CALCULATES Z AND DUROV POINTS *****
2220 REM
2230 FOR X=Z9 TO Z
2240 T=C(X)+D(X)+E(X)+F(X)
2250 IF T=0 THEN RETURN
2260 P(X)=(C(X)+D(X))/T*100
2270 P1(X)=(E(X)/T)*100
2280 P2(X)=(F(X)/T)*100
2290 T= G(X)+H(X)+K(X)
2300 P3(X)=(G(X)/T)*100

```

```

2310 P4(X)=(H(X)/T)*100
2320 P5(X)=(K(X)/T)*100
2330 L4=86.605-P4(X)*.86605\L5=50-.5773*L4
2340 L8=86.605+P2(X)*.5\L9=100+.86605*P2(X)
2350 W1(X)=(L9+50+(1.732*P(X)))/1.732
2360 W(X)=-.5773*L4+(50-P5(X))
2370 NEXT
2380 IF Q=1 THEN 2390 ELSE 2400
2390 CLOSE #1
2400 RETURN
2410 CLOSE #1\GOTO 900
2420 GOSUB 1150
2430 REM
2440 REM ** PRINTS DATA LINES USED IN DUROV PLOT ***
2450 REM
2460 !#1 CHR$(27),CHR$(140)
2470 !#1 CHR$(27), "U"
2480 !#1 CHR$(27), "D",CHR$(1),CHR$(80),CHR$(0)\!#1 CHR$(27),CHR$(15)
2490 !#1 CHR$(27), "- ",CHR$(1)\!#1 CHR$(9), ". ",CHR$(9), ". "
2500 !#1 CHR$(27), "D",CHR$(1),CHR$(10),CHR$(20),CHR$(30),CHR$(40),CHR$(50),
2510 !#1 CHR$(60),CHR$(70),CHR$(80)
2520 RESTORE 3140
2530 FOR X=1 TO 9
2540 READ R$,V
2550 IF V=9 THEN 2580
2560 !#1 CHR$(9),R$,
2570 GOTO 2590
2580 !#1 CHR$(9),R$
2590 NEXT
2600 !#1 CHR$(27), "- ",CHR$(0)
2610 !#1 CHR$(27), "D",CHR$(1),CHR$( 8),CHR$(18),CHR$(28),CHR$(38),CHR$(48),
2620 !#1 CHR$(60),CHR$(68),CHR$(78),CHR$(0)
2630 FOR X=1 TO 2
2640 !#1 CHR$(9),A(X),CHR$(9),B(X),CHR$(9),C(X),CHR$(9),D(X),CHR$(9),E(X),
2650 !#1 CHR$(9),F(X),CHR$(9),G(X),CHR$(9),H(X),CHR$(9),K(X)
2660 IF X=2 THEN 2670 ELSE 2680
2670 !#1 CHR$(27), "- ",CHR$(1)
2680 NEXT
2690 !#1
2700 !#1 CHR$(27), "- ",CHR$(0)
2710 RETURN
2720 END
2730 CLOSE#1\OPEN #1,B$
2740 HYBRID\VIEWPORT 0,99,20,119\GOSUB 1190\GOSUB 1260\GOSUB 1510
2750 REM
2760 REM ***** POINT BY RECORD # PLOT *****
2770 REM
2780 Z=0
2790 !\!
2800 !"INPUT RECORD # TO PLOT OR HIT(RETURN) FOR SERVICE MENU "
2810 INPUT F$\IF LEN(F$)=0 THEN 2900 \D=VAL(F$)
2820 IF INT(D)<1 OR INT(D)>5 THEN 2830 ELSE 2850
2830 !"YOU INPUT AN OUT OF BOUNDS ROW # "
2840 !"-----"\GOTO 2790
2850 Z=Z+1\Z9=Z
2860 D1=(D-1)*45

```

```

2870 READ #1 ZD1,A(Z),B(Z),C(Z),D(Z),E(Z),F(Z),G(Z),H(Z),K(Z)
2880 GOSUB 2230\POINT W1(Z),W(Z)
2890 GOTO 2790
2900 CLOSE #1\TEXT\GOTO 910
2910 REM
2920 REM ***** ASKS IF PLOT BE SECTIONED INTO FOUR QUADRANTS ***
2930 REM
2940 INPUT "DO YOU WANT THE PLOT SECTIONED ",A$
2950 !CHR$(4)
2960 !"IF YOU WISH A HARDCOPY OF DUROV PLOT.WAIT FOR PLOT COMPLETION,"
2970 !"THEN PRESS CONTROL T "\FOR I=1 TO 4500\NEXT
2980 RETURN
2990 REM ***** PRINTS ZION COCENTRATIONS *****
3000 REM
3010 FOR X=1 TO 2
3020 !#1 Z31,A(X),Z10F2,P(X),P1(X),P2(X),P3(X),P4(X),P5(X)
3030 NEXT
3040 RETURN
3050 REM ***** PRINTS HEADLINES FOR ZION CONCENTRATIONS *****
3060 REM
3070 !#1 CHR$(27),CHR$(140)
3080 !#1 CHR$(27),"D",CHR$(1),CHR$(9),CHR$(19),CHR$(29),CHR$(39),CHR$(49),
3090 !#1 CHR$(59),CHR$(0)!\#1 CHR$(27),"-",CHR$(1)
3100 !#1 CHR$(9),"ID#",CHR$(9),"ZNa+K",CHR$(9),"ZCa",CHR$(9),"ZMg",
3110 !#1 CHR$(9),"ZHCO3",CHR$(9),"ZSO4",CHR$(9),"ZCl"
3120 !#1 CHR$(27),"-",CHR$(0)
3130 RETURN
3140 DATA "ID#",1,"DATE",2,"Na",3,"K",4,"Ca",5,"Mg",6,"ALKAL",7,"SO4",8,"Cl",9
3150 REM
3160 REM ***** THIS SECTION COUNTS # OF LINES IN DATA IN FILE *****
3170 REM
3180 OPEN #1,B$
3190 D5=0
3200 IF TYP(1)=0 THEN RETURN
3210 READ #1,A,B,C,D,E,F,G,H,K
3220 IF A=2.020202E-33 THEN RETURN
3230 D5=D5+1
3240 GOTO 3200
3250 REM
3260 REM ***** THIS SECTION CHECKS FOR OUT OF BOUNDS COL# *****
3270 REM
3280 IF INT(N9)<1 OR INT(N9)>9 THEN A$="N"\RETURN

```